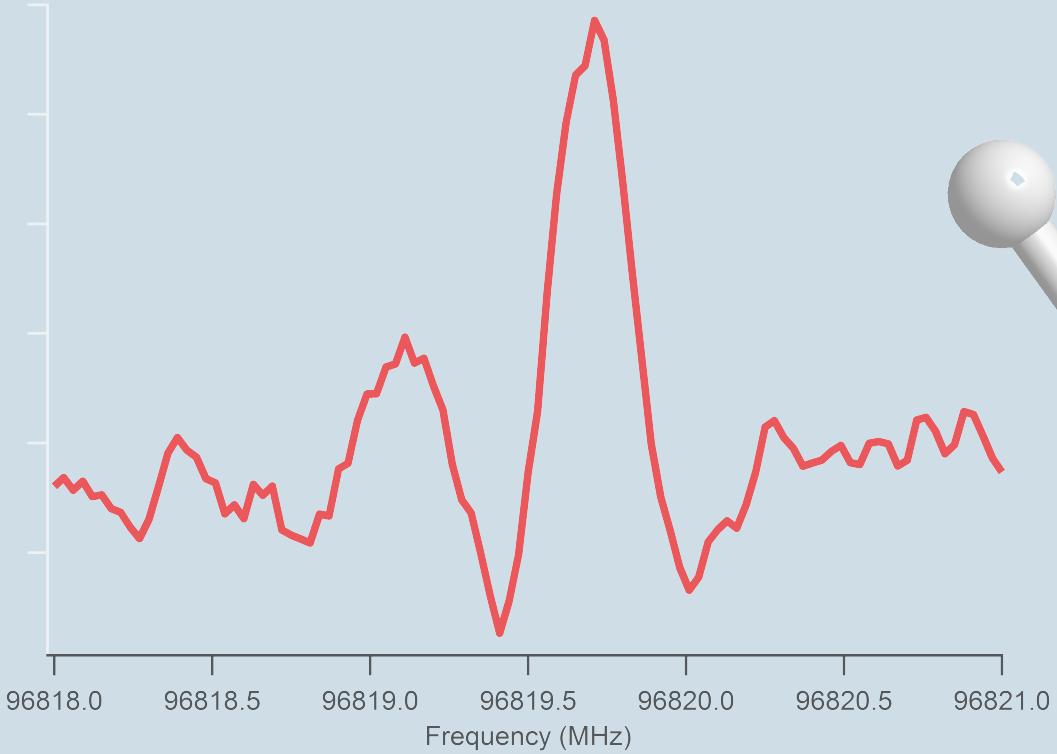
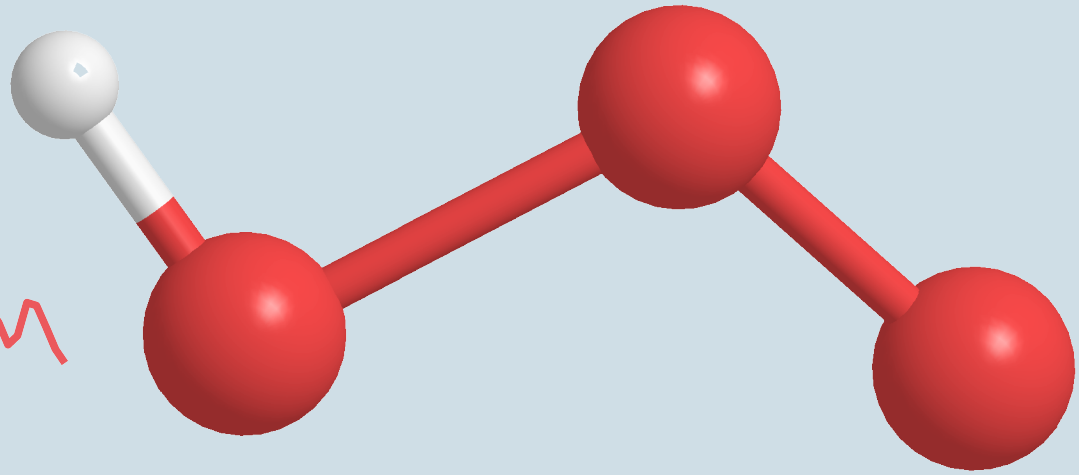
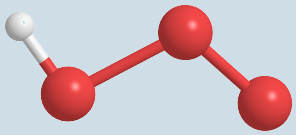




MILLIMETER AND SUBMILLIMETER SPECTROSCOPIC STUDIES OF HO_3

Luyao Zou, Susanna L. Widicus Weaver

Department of Chemistry, Emory University, Atlanta, GA, USA



WHY HO_3 ?

G eometry

S pectroscopy

B ond Strength

A strochemistry

GEOMETRY

Central O-O bond length

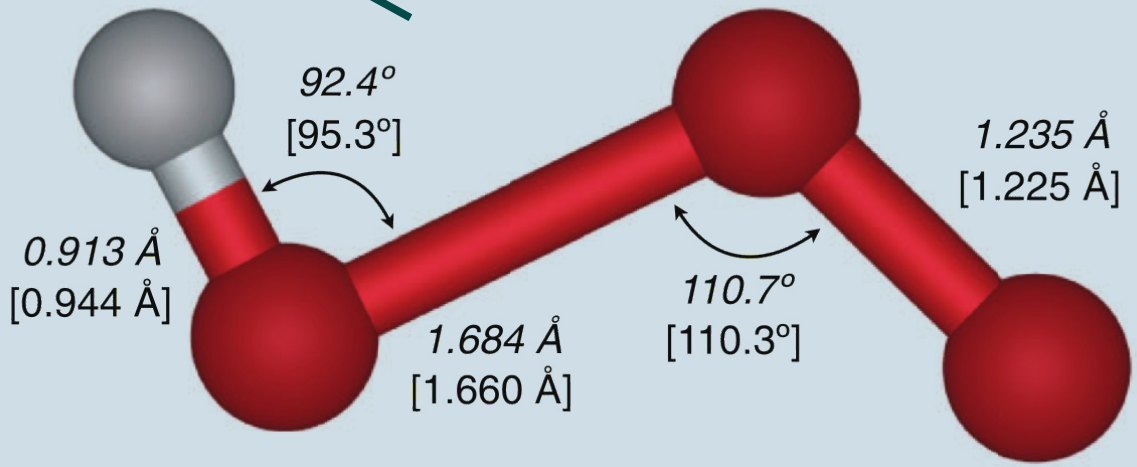
Experimental

Suma	1.688
McCarthy	1.684

Calculation

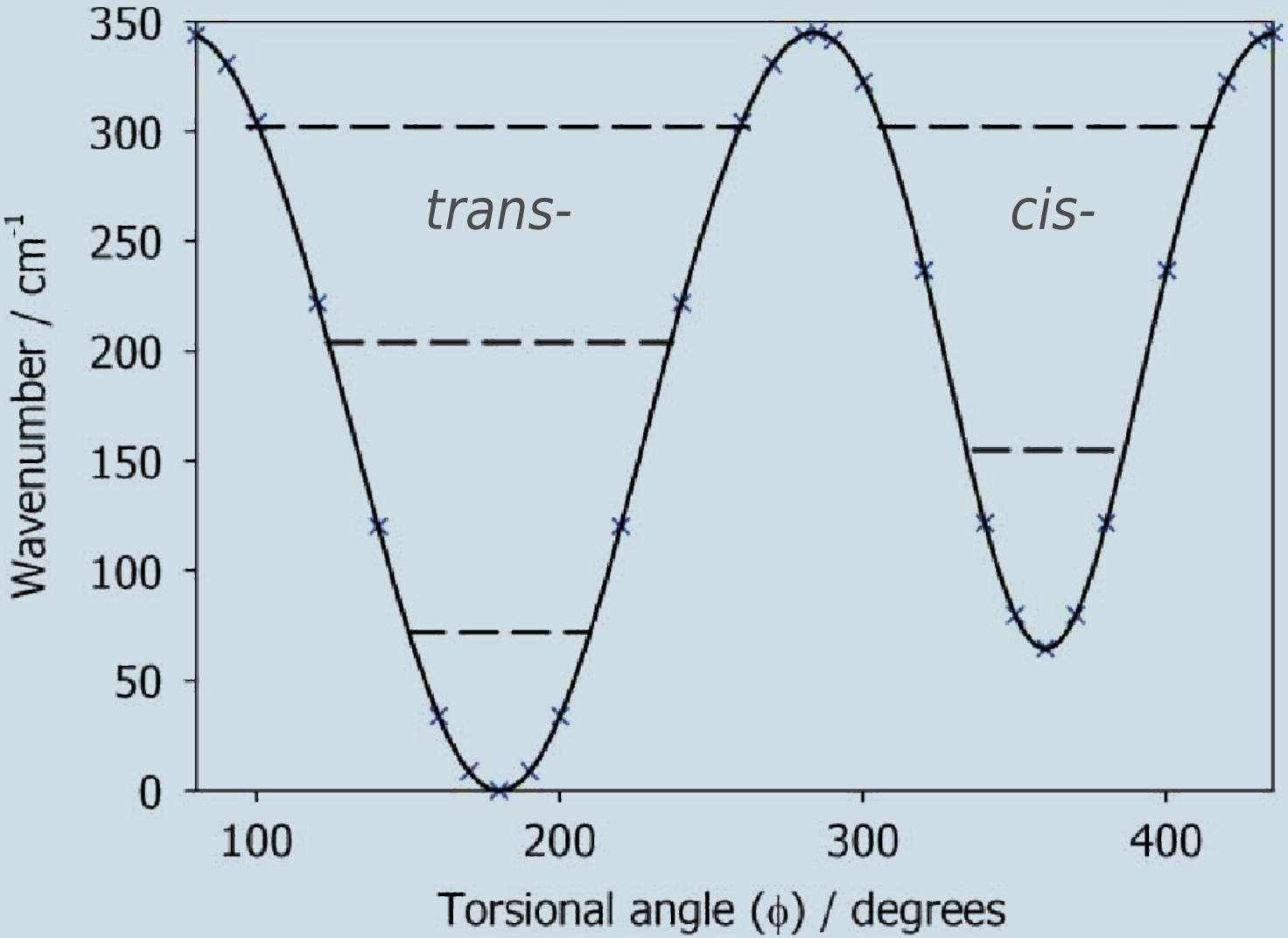
Hoy	1.618
Denis	~ 1.5
Varandas	~ 1.42

Planar



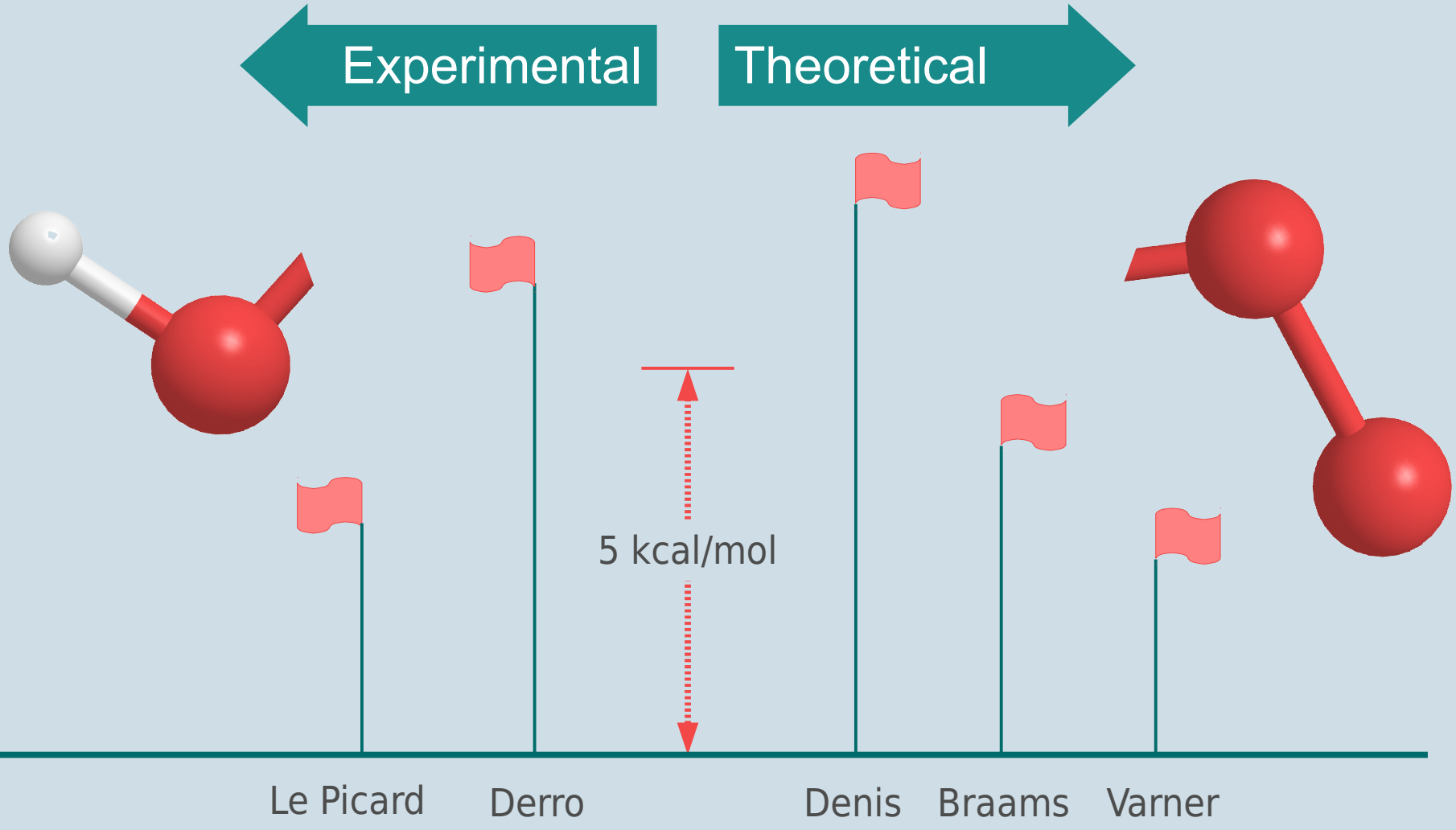
Varandas, A. J. C. et al., Molecular Physics, 1997
Denis, P. A. et al., Chem. Phys. Lett., 2002
Suma, K. et al., Science, 2005
McCarthy, M. C. et al., J. Chem. Phys., 2012
Hoy, E. P. et al., J. Phys. Chem. A, 2013

Torsion & Isomerization

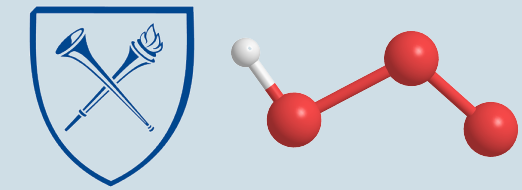


Beames, J. M. et al., J. Chem. Phys., 2011

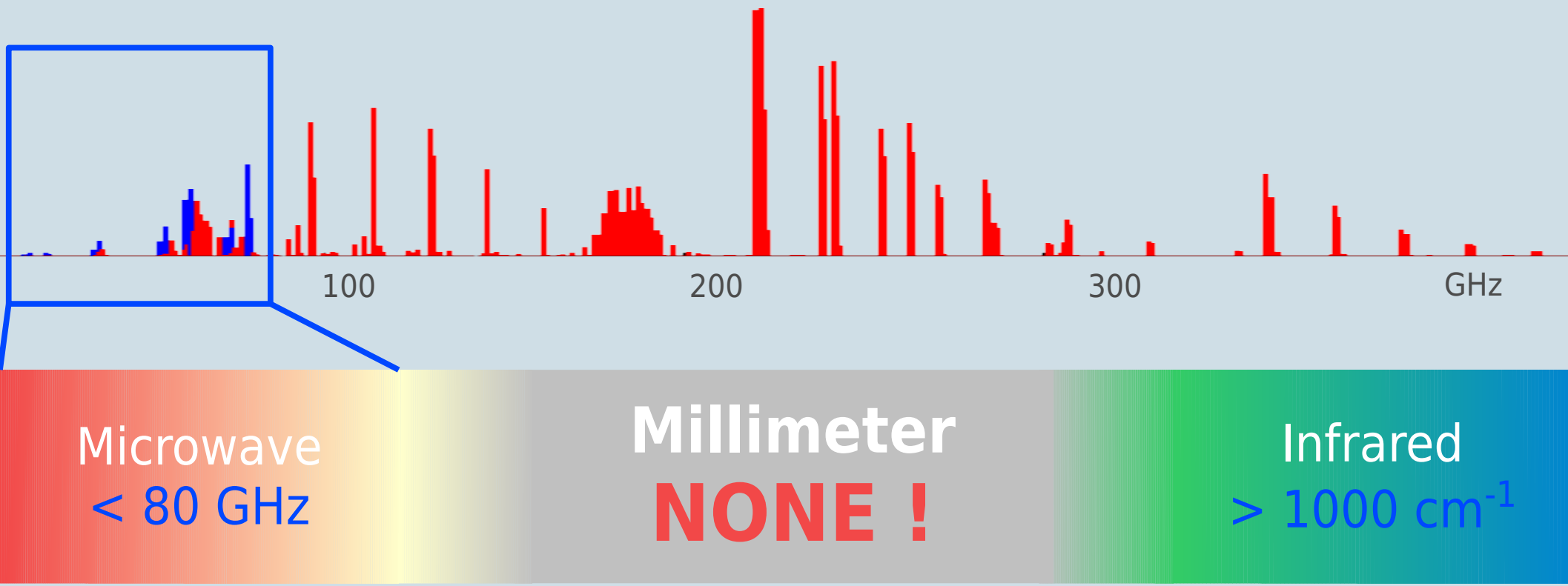
DISSOCIATION LIMIT



Braams, B. J. et al., Phys. Chem. Chem. Phys., 2008.
Derro, E. L. et al., J. Phys. Chem. A, 2008
Denis, P.A. et al., J. Phys. Chem. A, 2009
Varner, E. et al., J. Phys. Chem. A, 2009
Le Picard, S. D. et al., Science, 2010



MEASURED TRANSITIONS



Microwave
< 80 GHz

Millimeter
NONE !

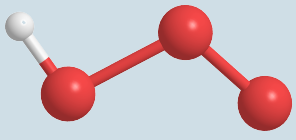
Infrared
> 1000 cm^{-1}

Does HO_3 EXIST in the Interstellar Medium ?

Grain surface reaction in dark clouds leads to O_2 depletion. HO_3 may have a chance to form in the grain surface. However, no one has identified HO_3 in space.

Orion & Horsehead Nebular
Credit: Roberto Colombari & Federico Pelliccia, NASA Astronomy Picture of the Day

Hincelin, U. et al., Astron. & Astrophys., 2011

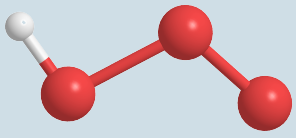


THIS study

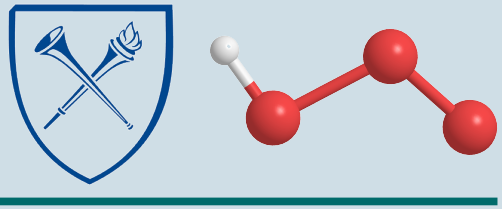
L INES!

P arameters

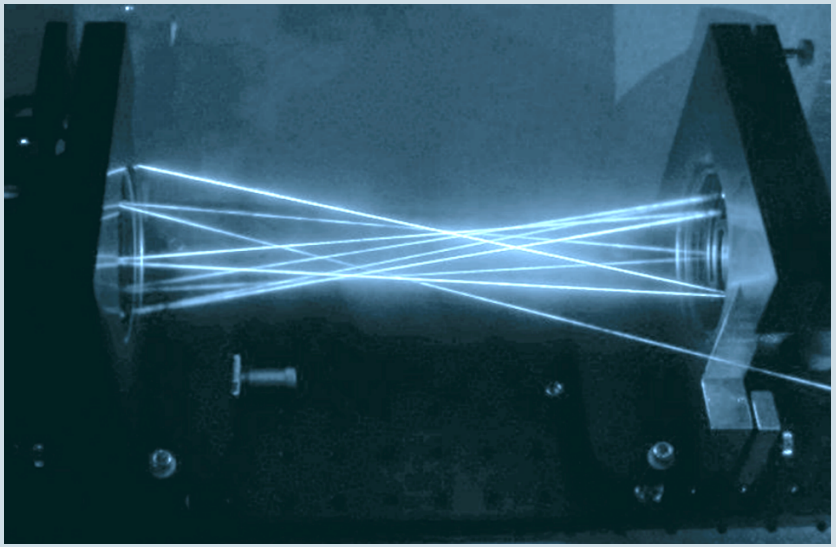
S upport for Astrochemistry



THE **EXPERIMENT**



Vacuum
Chamber
Multiplier
Chain
x 3-9
Pulsed Valve +
Discharge Source
Multipass
Beam
Detector
Synthesizer
Lock-in
Oscilloscope
To computer
Trigger
Delay
Generator
High Voltage Pulse
Generator
Gate
High Voltage
Power Supply
Pulse Valve
Driver

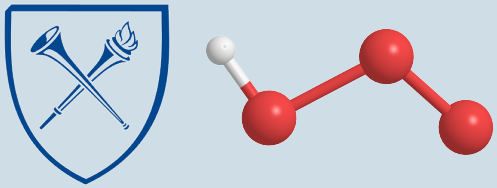


Direct Absorption Spectrometer with

MULTIPASS

Optical Design

Laas, J. C. et al., J. Phys. Chem. A, 2013



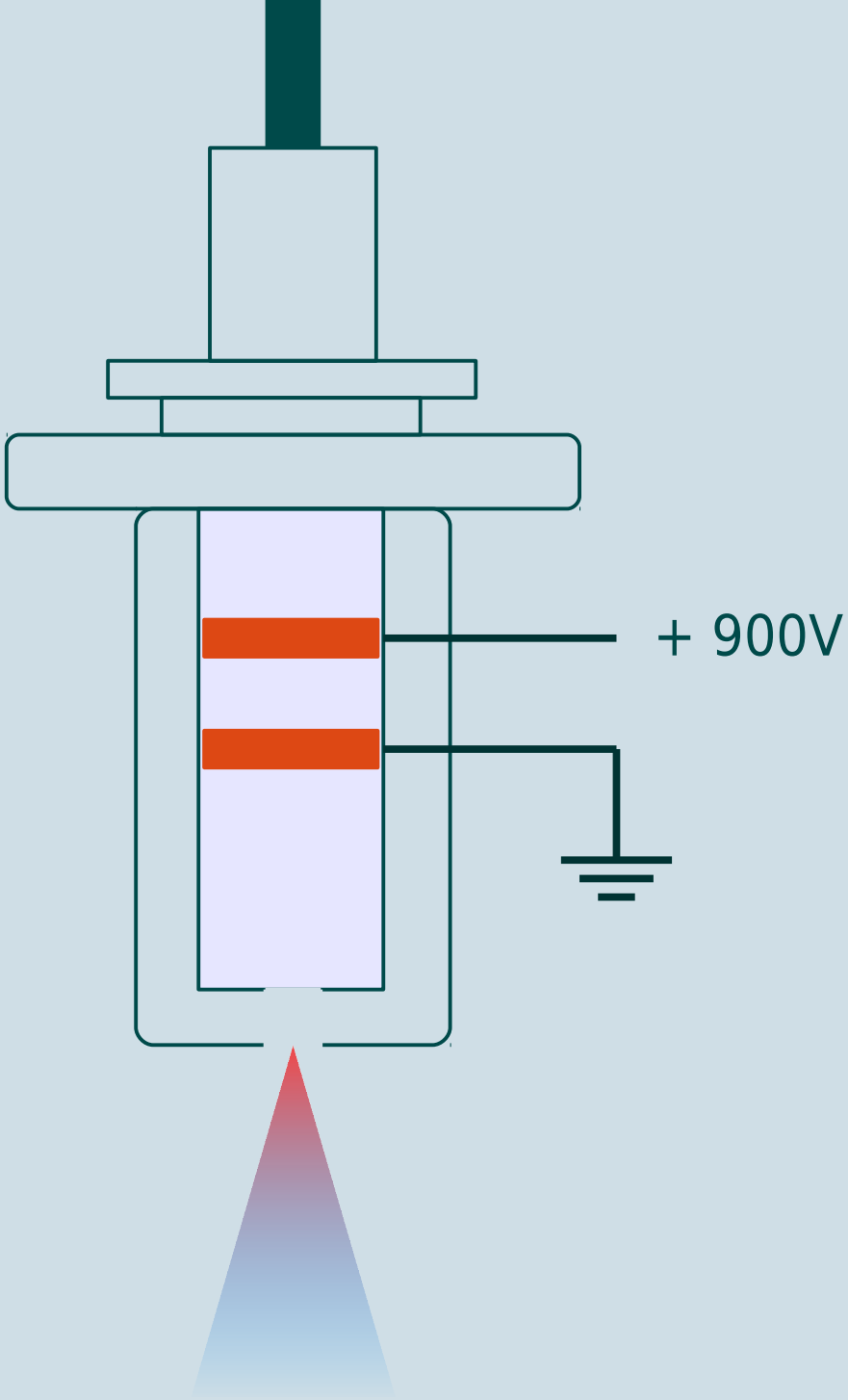
PULSED
Discharge Source

TRIGGERED by
the pulsed valve

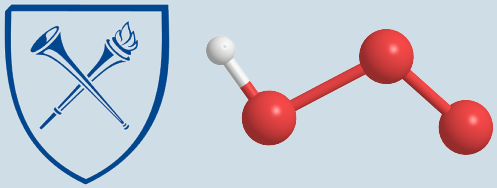
SUPERSONIC
Expansion

COOLS the radical down to
15 K rotational temperature

INCREASES line intensity

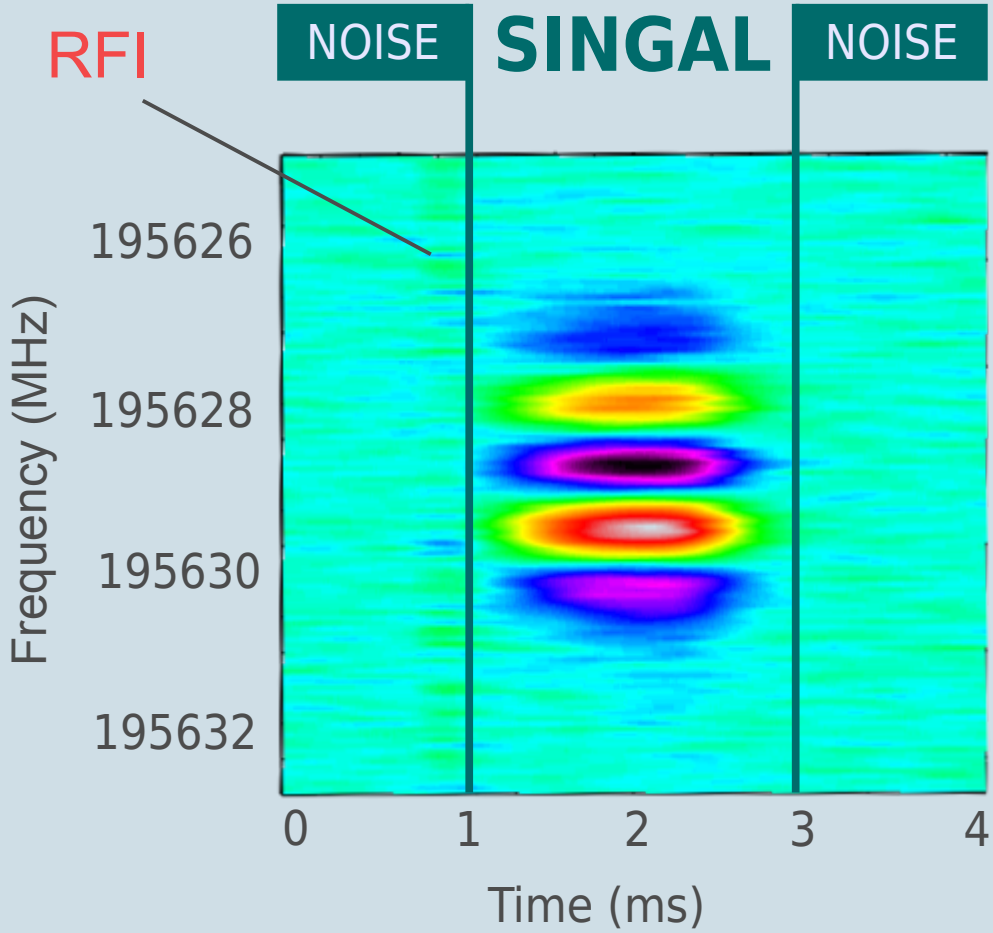


McCarthy, M. C. et al., Astrophys. J. S, 2000



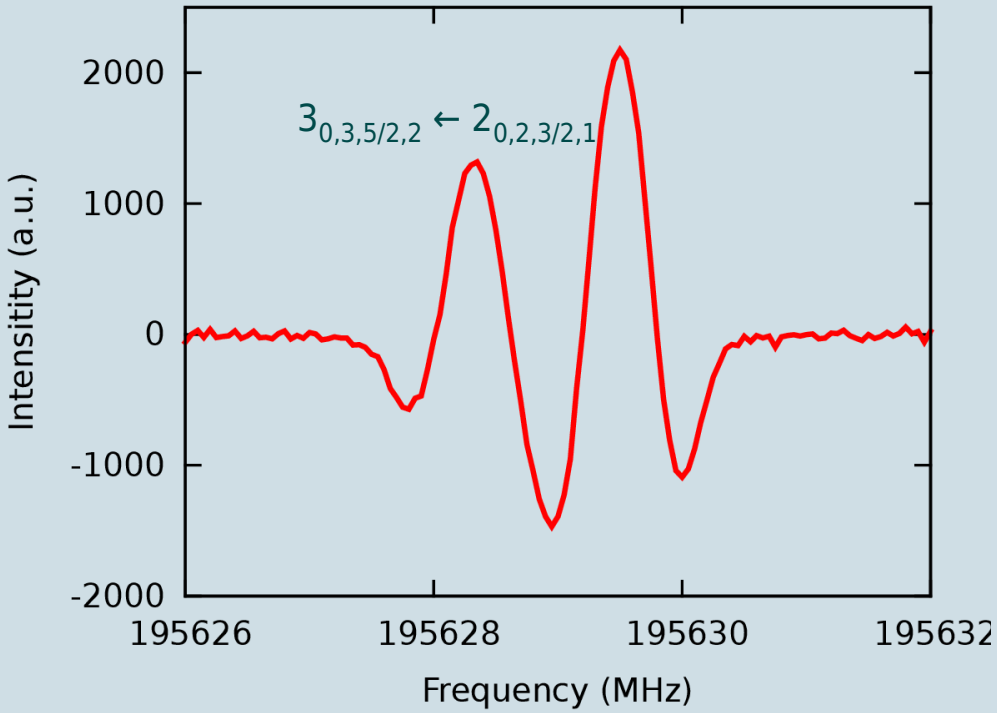
BOXCAR
Integration

HO_2 lines as an EXAMPLE

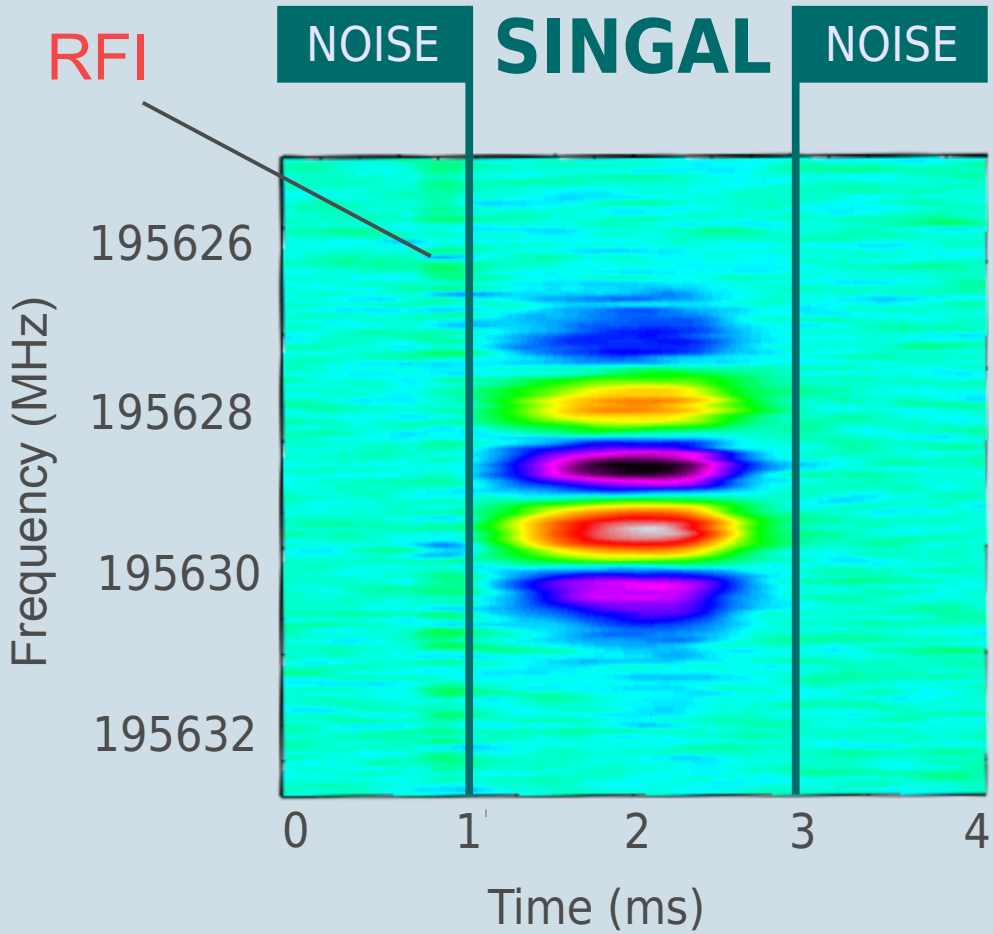


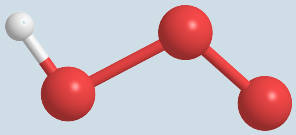
BOXCAR
Integration

HO_2 lines as an EXAMPLE

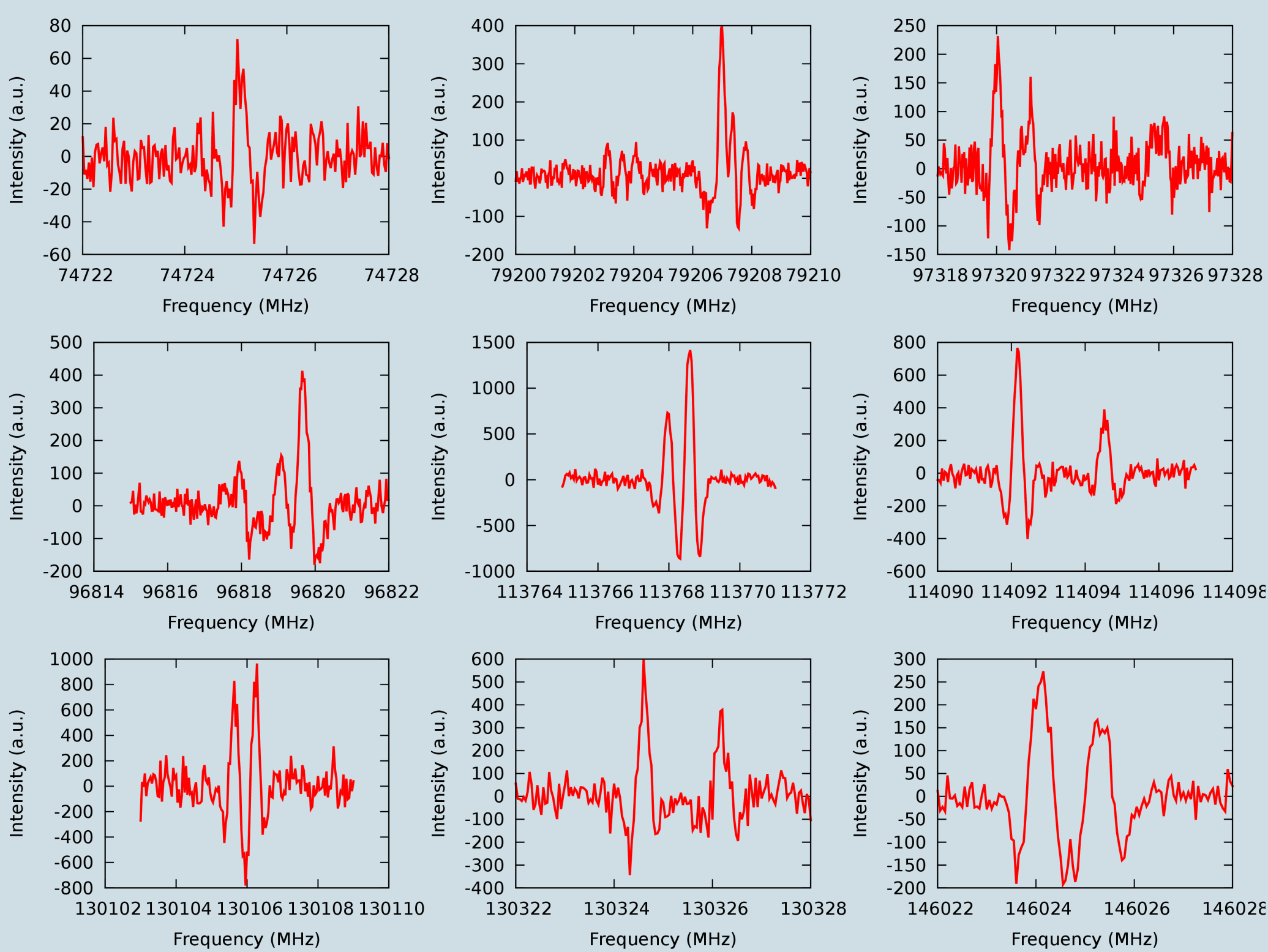


HO_2 transition observed readily in discharge

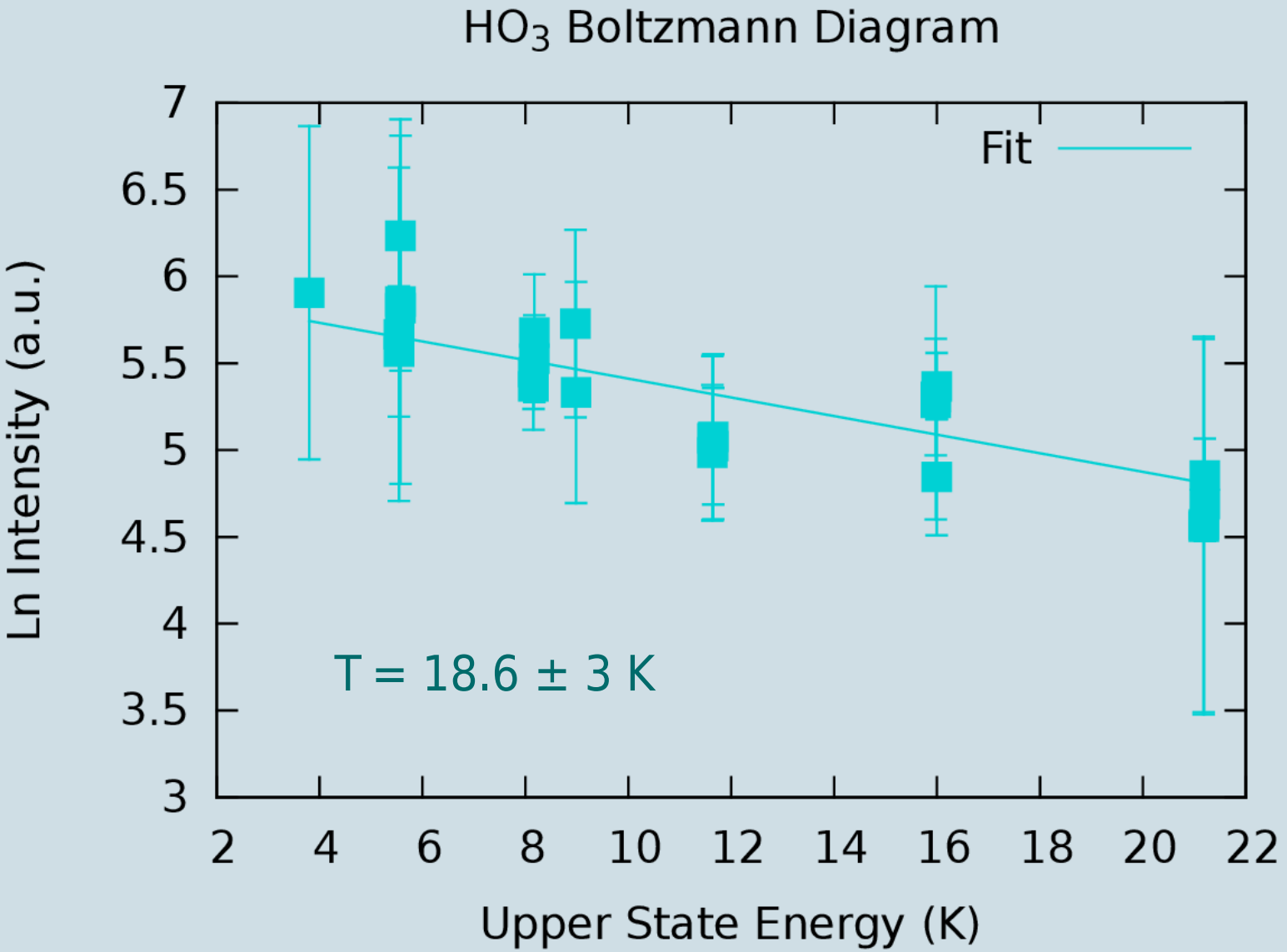


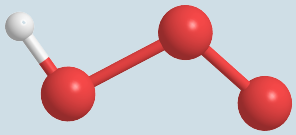


THE HO_3 LINES


Intensity (a.u.)
Frequency (MHz)
80
60
40
20
0
-20
-40
-60
74722
74724
74726
74728
400
300
200
100
0
-100
-200
79200 79202 79204 79206 79208 79210
250
200
150
100
50
0
-50
-100
-150
97318 97320 97322 97324 97326 97328
500
400
300
200
100
0
-100
-200
96814 96816 96818 96820 96822
1500
1000
500
0
-500
-1000
113764 113766 113768 113770 113772
800
600
400
200
0
-200
-400
-600
114090 114092 114094 114096 114098
1000
800
600
400
200
0
-200
-400
-600
-800
130102 130104 130106 130108 130110
600
500
400
300
200
100
0
-100
-200
-300
-400
130322 130324 130326 130328
300
250
200
150
100
50
0
-50
-100
-150
-200
146022 146024 146026 146028

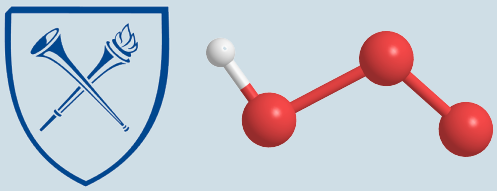
PROBING **TEMPERATURE**



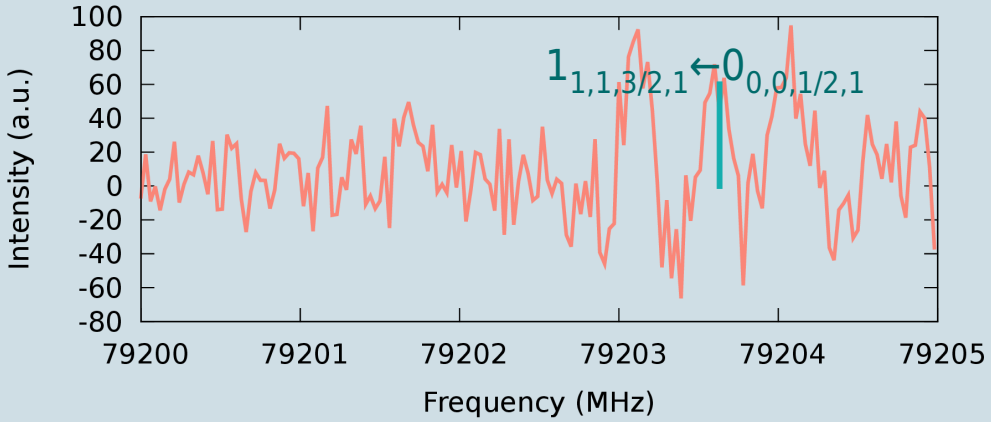


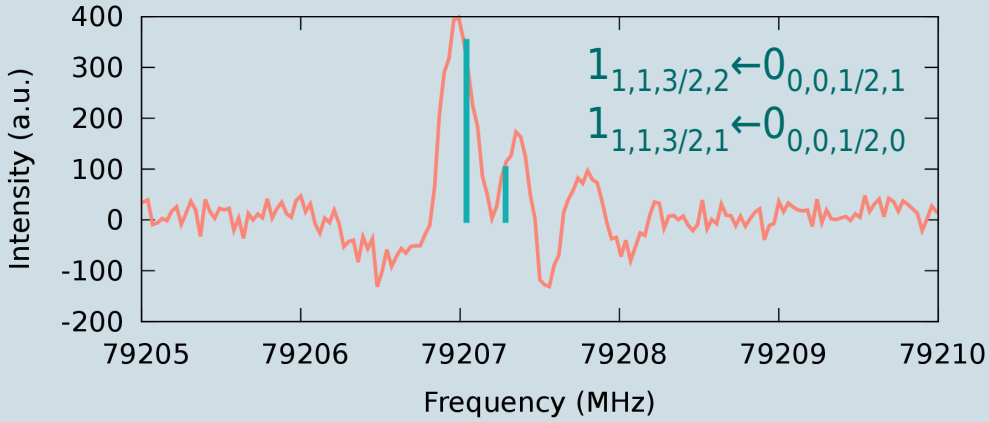
FITTING RESULTS

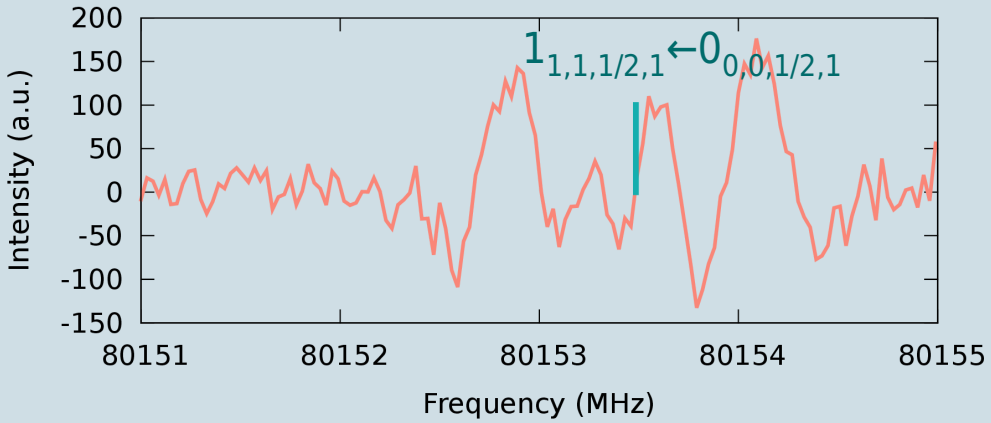
Parameters	Suma et al.	This study
A-(B+C)/2	61409.61111(172)	61409.61043(169)
(B+C)/2	9368.55408(46)	9368.55403(45)
(B-C)/4	309.19802(39)	309.19756(34)
Δ_N	0.0464608(242)	0.0464512(235)
Δ_{NK}	0.15335(32)	0.153158(308)
δ_N	0.006108(33)	0.0060665(281)
ε_{aa}	-1252.5858(47)	-1252.5858(46)
ε_{bb}	-106.25509(207)	-106.25513(205)
ε_{cc}	-3.49541(193)	-3.49515(192)
$\lvert\varepsilon_{ab} + \varepsilon_{ba}\rvert/2$	42.450(85)	42.457(84)
Δ_N^S	0.000998(82)	0.0001011(80)
Δ_{NK}^S	0.05441(122)	0.05449(120)
a_F	3.65871(243)	3.65869(243)
$1.5T_{aa}$	12.7242(71)	12.7233(71)
$0.25(T_{bb} - T_{cc})$	-1.30597(237)	-1.30628(236)

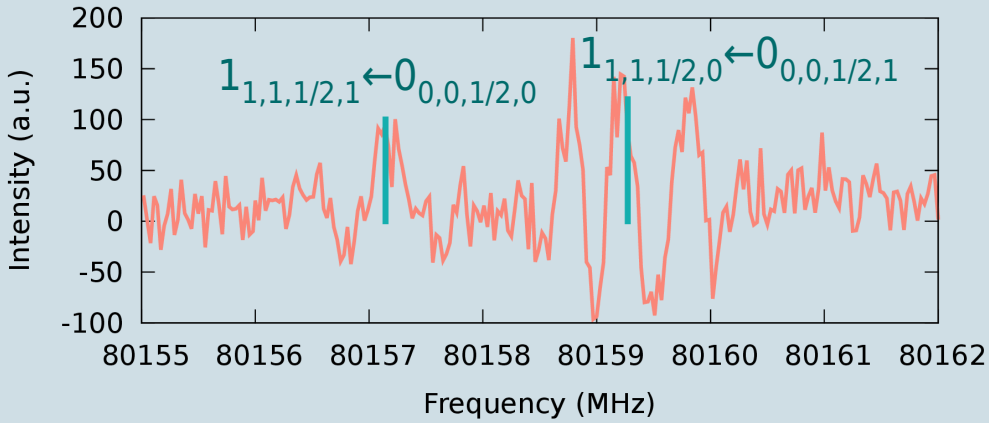


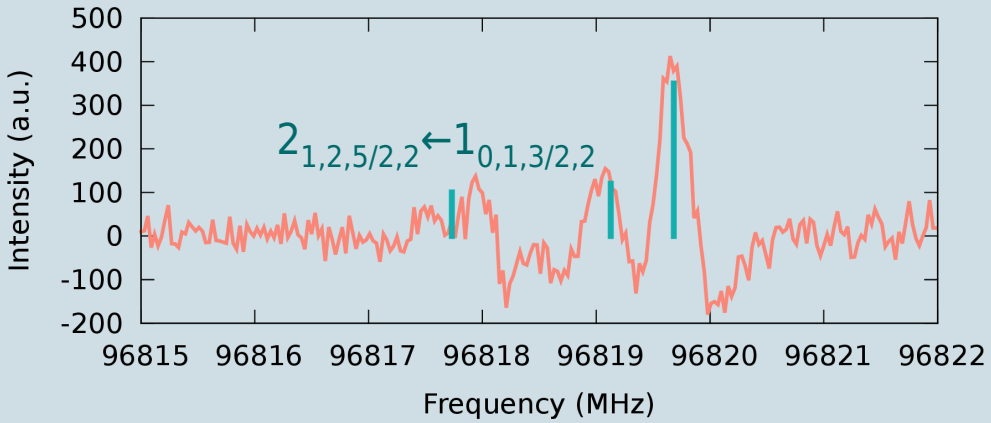
UNEXPECTED SPLITTING

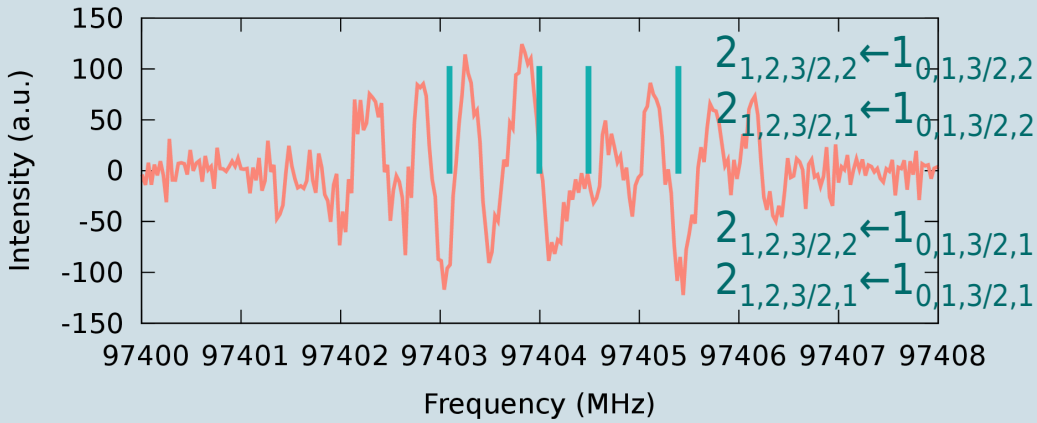


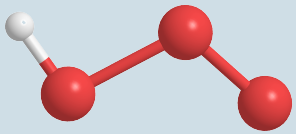






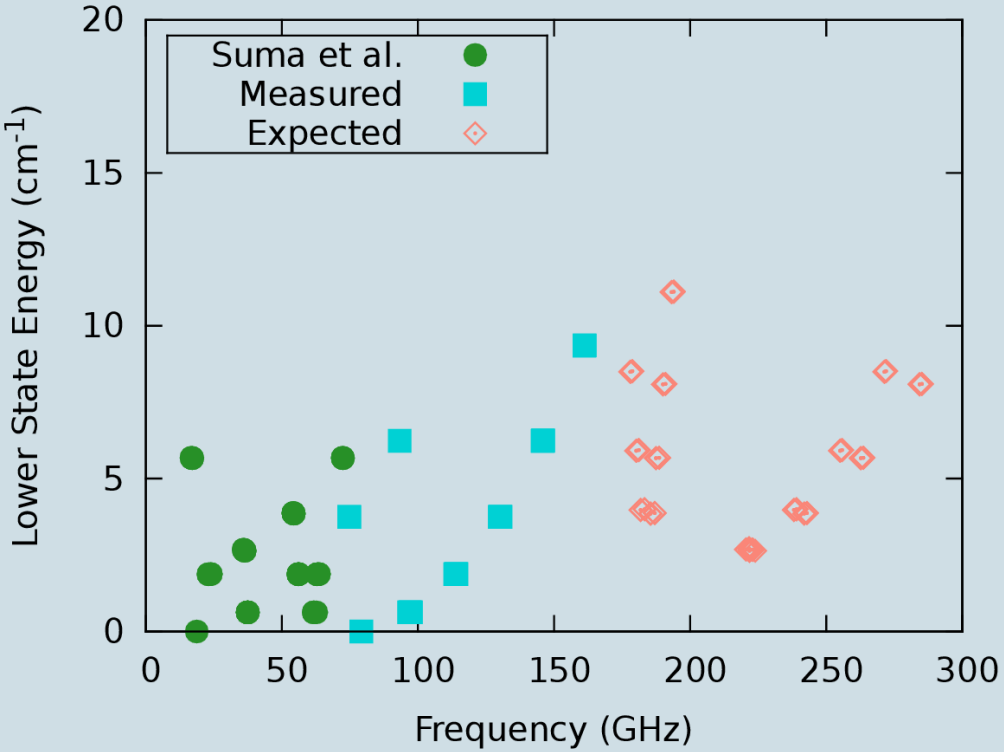


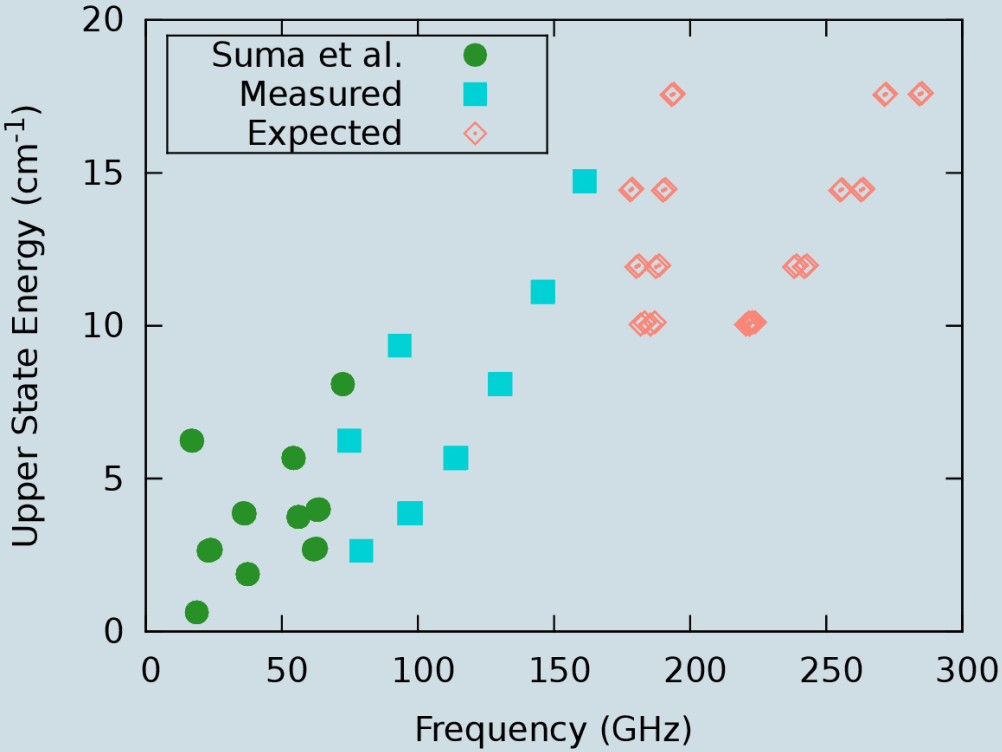


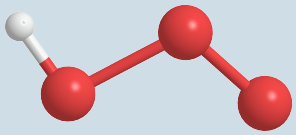


UNABLE TO SEE MORE LINES

Power Drop **OR** Torsion **OR** ? ? ?







NEW LINES

>25 new lines of HO_3 are observed in the laboratory from 70 to 162 GHz up to J=6

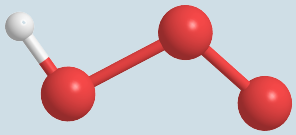
FITS

Preliminary fits are conducted. 15 parameters are refined

PUZZLES

Unexpected splitting pattern at low frequencies
Unable to see more lines

IN SUMMARY



What's NEXT

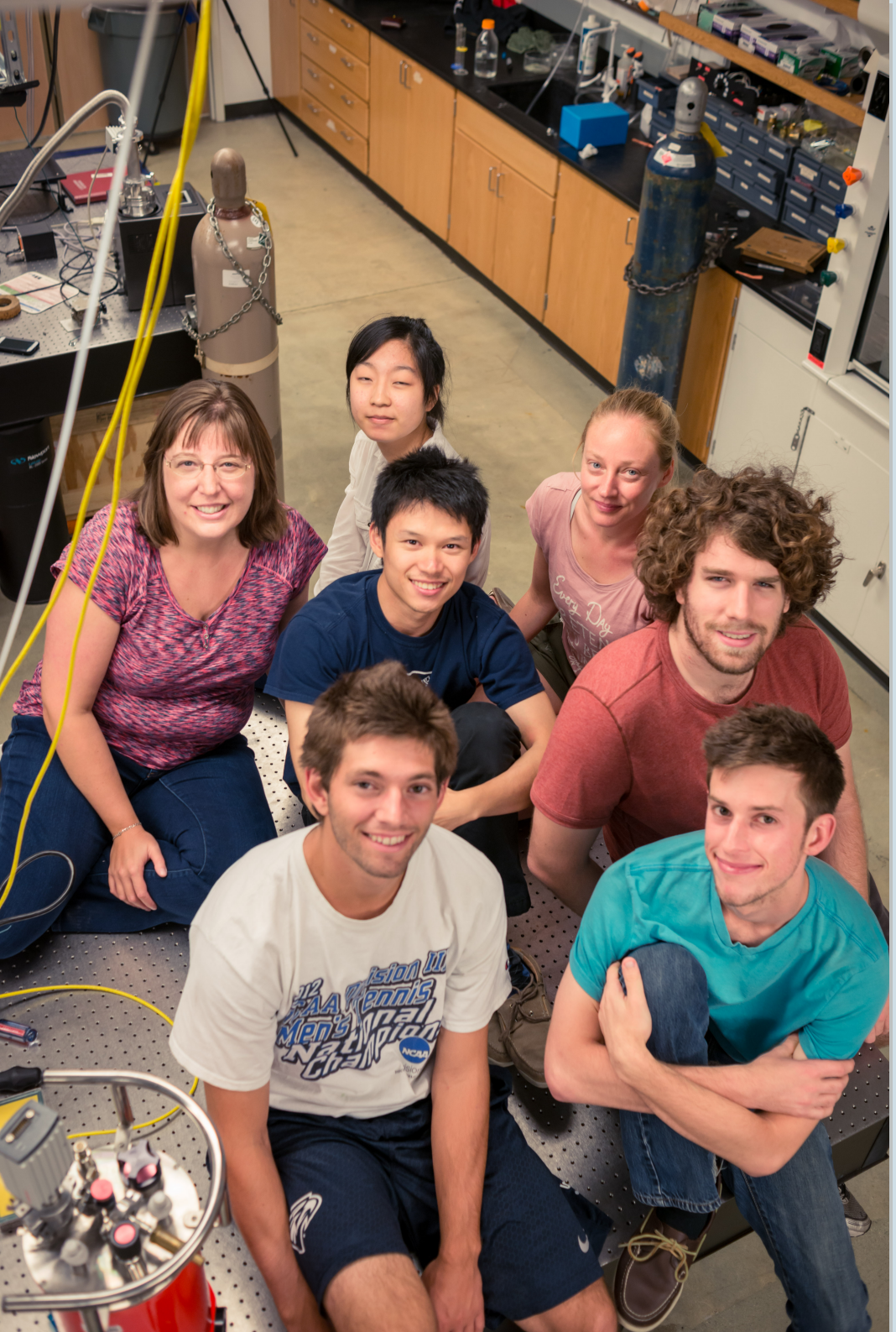
INCREASE spectrometer power

REPEAT with DO_3 to determine source of spectral splitting

ADD Helmholtz coils

EXTEND measurements to higher frequencies

COMPARE results to observations



ACKNOWLEDGEMENT

The Widicus Weaver Group
Mike McCarthy
NSF and Emory University for $$$